

# **The role of bay breezes on a high surface ozone episode during the Houston, Texas DISCOVER-AQ field campaign**

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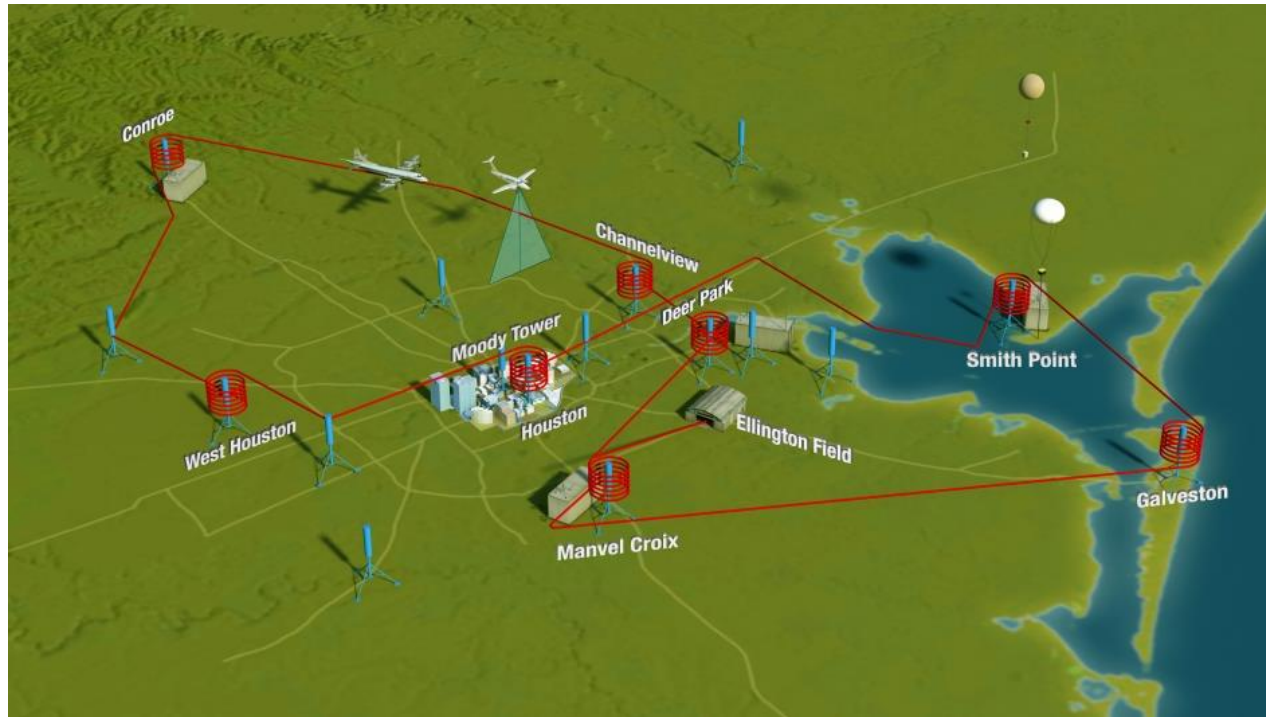
September 3, 2015

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# Introduction

- High air pollution event occurred on September 25, 2013 during the DISCOVER-AQ Houston, Texas field deployment.
- Sea and bay breezes took place during this event.
- Possible over-assisted flaring events from petrochemical facilities observed during this event.

# DISCOVER-AQ (Deriving Information on Surface conditions from Column and VERTically resolved observations relevant to Air Quality)

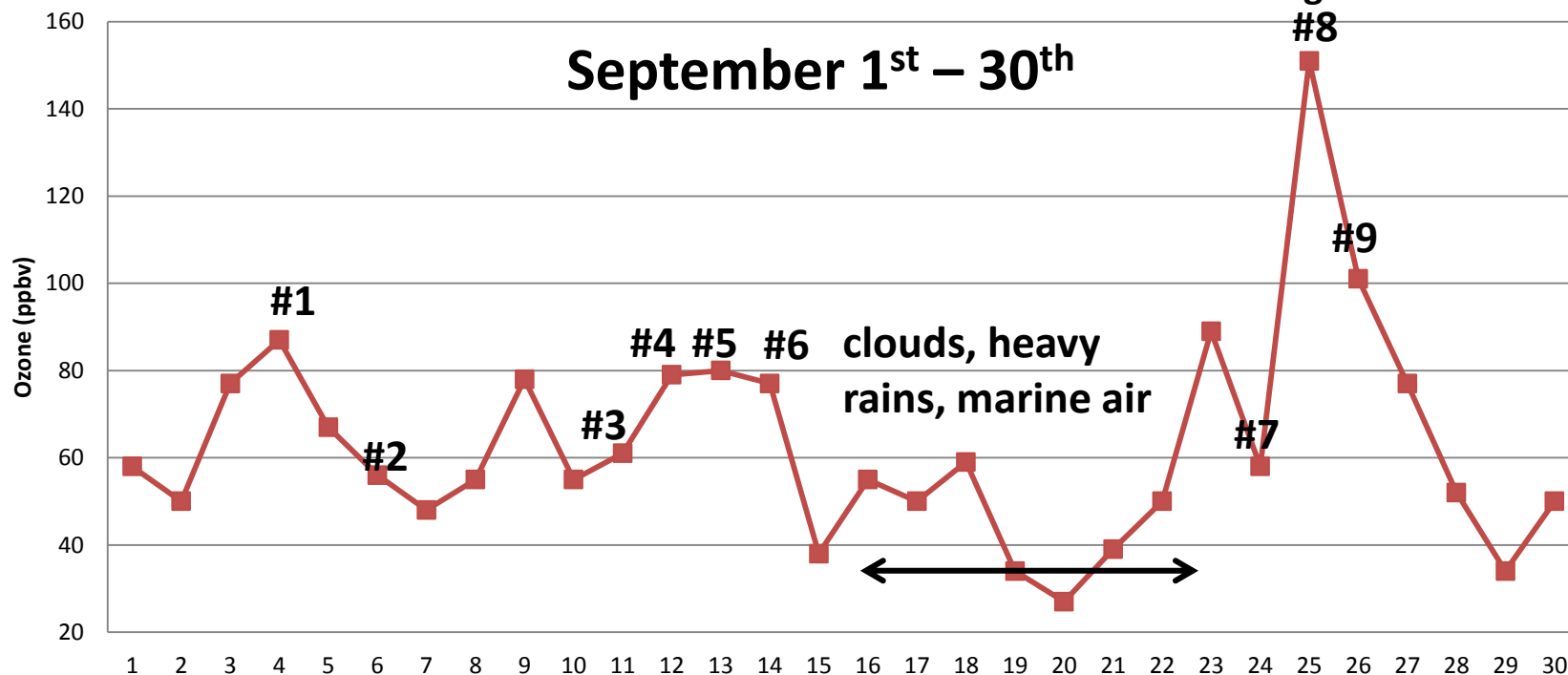


- Houston deployment: September 2013
- 9 flight days conducting spirals and missed approaches throughout the Houston metropolitan area.
- Numerous other ground-based measurements (Pandora UV/Vis spectrometers, AERONET sunphotometers, in-situ stationary and mobile platforms, ozonesondes, and tethersondes).

# Daily 1-Hour Max Ozone (ppbv) – All Stations

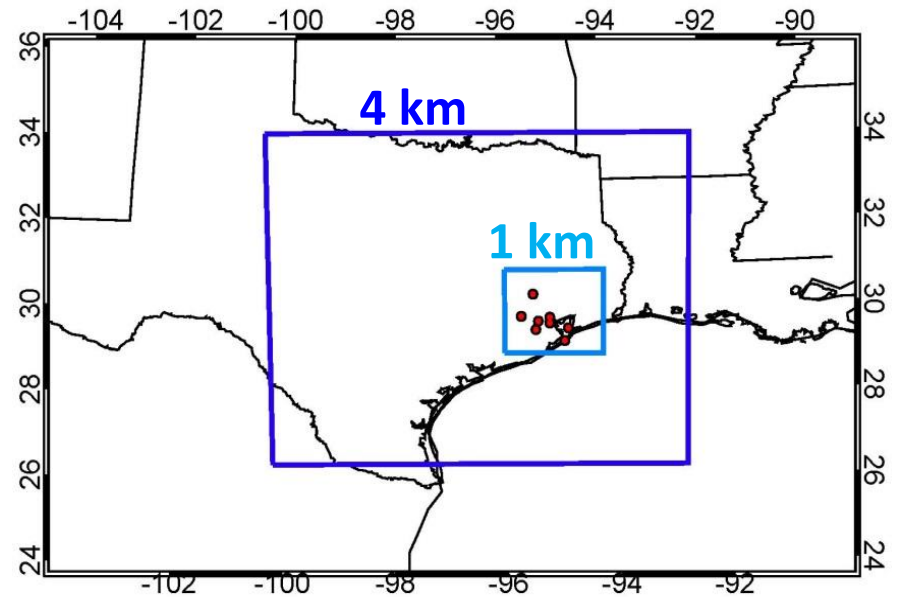
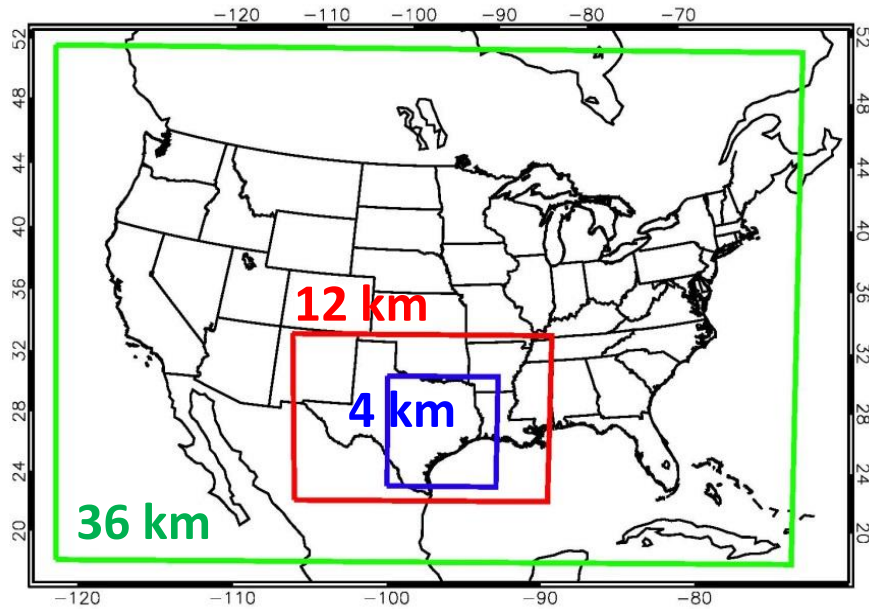
Daily 1-Hour Max Ozone (ppbv)

bay, sea breezes  
following cold front



- Onshore flow during most of the campaign
- September 25 was the exception
  - Northerly transport into Houston
  - Sea and bay breezes caused pollutants to recirculate
  - Peak surface ozone near Galveston Bay
  - 1 hour max: 151 ppbv
  - 8 hour max: 124 ppbv

# WRF/CMAQ Domains



## **Weather Research and Forecasting (WRF) Version 3.6.1 Model Options**

Radiation	LW: RRTM; SW: Goddard
Surface Layer	Pleim-Xiu
Land Surface Model	Pleim-Xiu
Boundary Layer	ACM2
Cumulus	Kain-Fritsch
Microphysics	WSM-6
Nudging	Observational and analysis nudging
Damping	Vertical velocity and gravity waves damped at top of modeling domain
SSTs	Multi-scale Ultra-high Resolution (MUR) SST analysis (~1 km resolution)

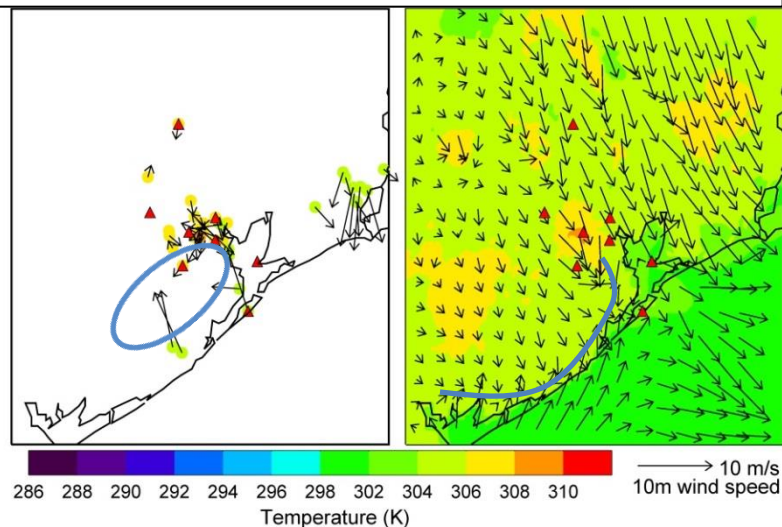
## **CMAQ Version 5.0.2 Model Options**

Chemical Mechanism	CB05
Aerosols	AE5
Dry deposition	M3DRY
Vertical diffusion	ACM2
Emissions	2012 TCEQ anthropogenic emissions BEIS calculated within CMAQ
Initial and Boundary conditions	MOZART CTM

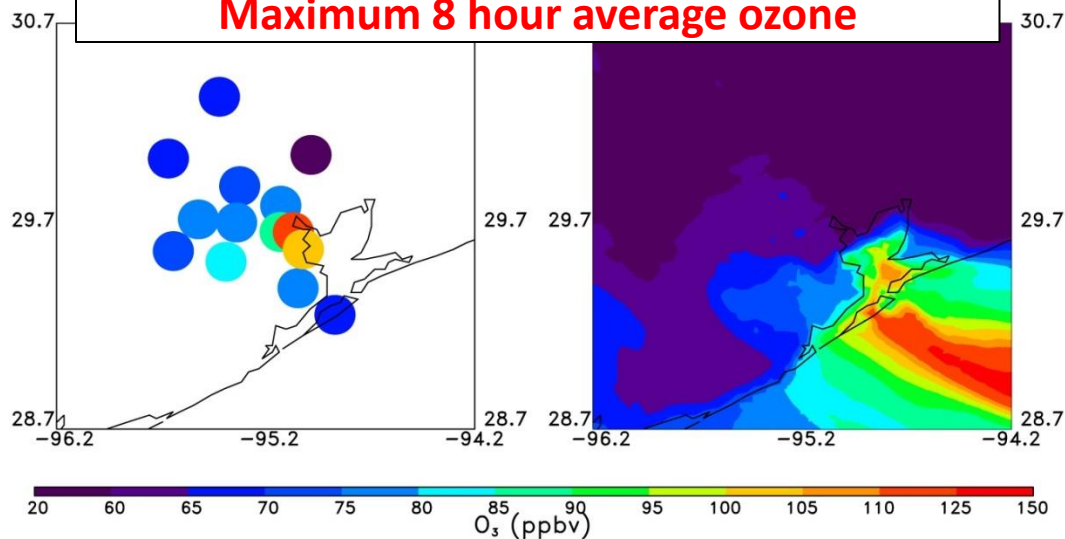
# WRF simulations

- Time period:
  - 18 August – 2 October, 2013
- **Original simulation (4 km domain only)**
  - Initial and boundary conditions – 40 km NARR
  - WRF reinitialized every three days
    - Run in 3.5 day increments, with the first 12 hours discarded
  - Observational and analysis nudging on 36 km domain only
  - Output saved hourly

**2m temperature 10 m wind velocity**



**Maximum 8 hour average ozone**



- WRF simulated weaker sea and bay breezes than observed
- Model biased low for surface ozone

# WRF simulations

- Time period:
  - 18 August – 2 October, 2013
- **Original simulation (4 km domain only)**
  - Initial and boundary conditions – 40 km NARR
  - WRF reinitialized every three days
    - Run in 3.5 day increments, with the first 12 hours discarded
  - Observational and analysis nudging on 36 km domain only
  - Output saved hourly
- **Iterative runs (EPA Method) (4 km and 1 km domains)**
  - Initial and boundary conditions – 12 km NAM
  - Observational nudging of all domains
  - 1 km nonpoint emissions interpolated from 4 km emissions
  - Output saved every 20 minutes (4 km) and 5 minutes (1 km)
  - *Iteration #1*
    - Analysis nudging on all domains based on 12 km NAM
  - *Iteration #2*
    - 4 and 1 km domains: analysis nudging of 2 m temperature and humidity from previous WRF run, everything else from 12 km NAM

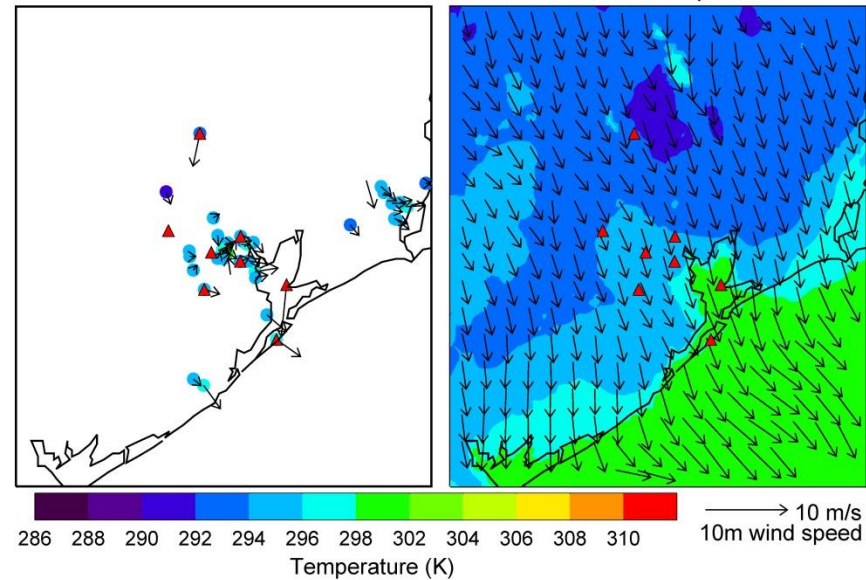


# September 25

2013-09-25 12 Z \_iter2

Observations

MCIP 2M Temperature



6 am CST:

Observations – calm  
winds

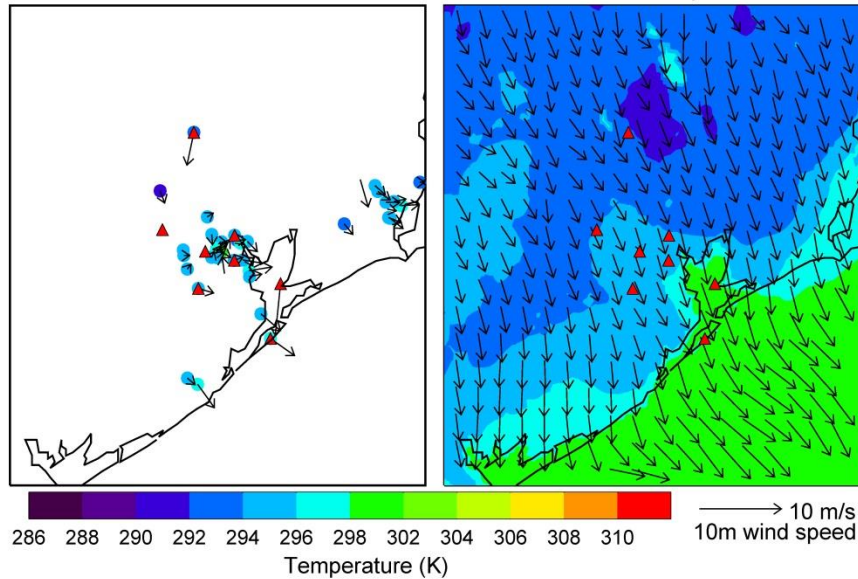
Model – weak  
northwesterly  
transport into Houston

# September 25

2013-09-25 12 Z \_iter2

Observations

MCIP 2M Temperature



6 am CST:

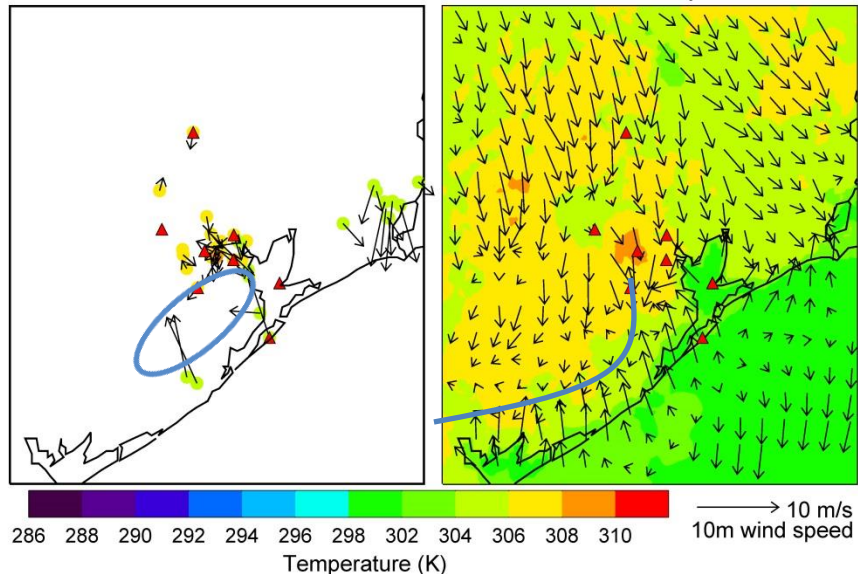
Observations – calm winds

Model – weak northwesterly transport into Houston

2013-09-25 21 Z \_iter2

Observations

MCIP 2M Temperature

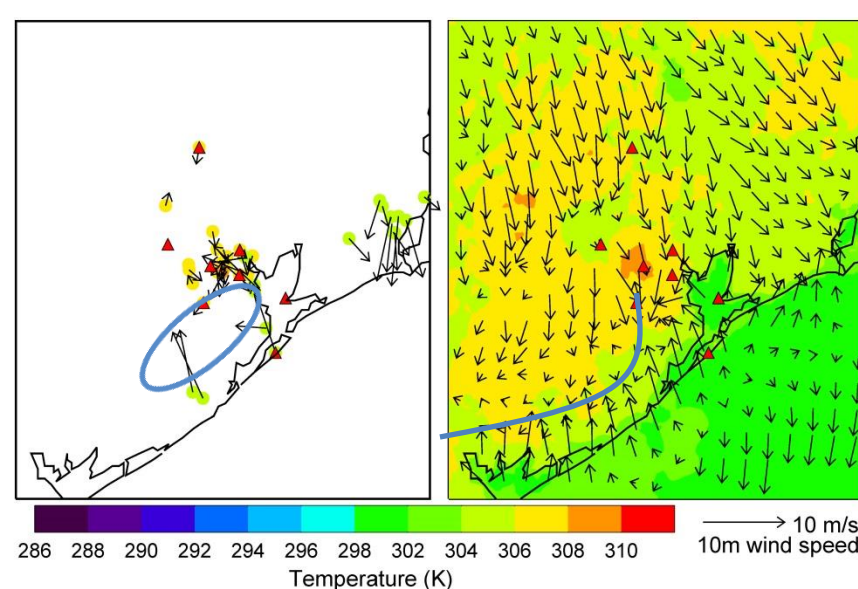
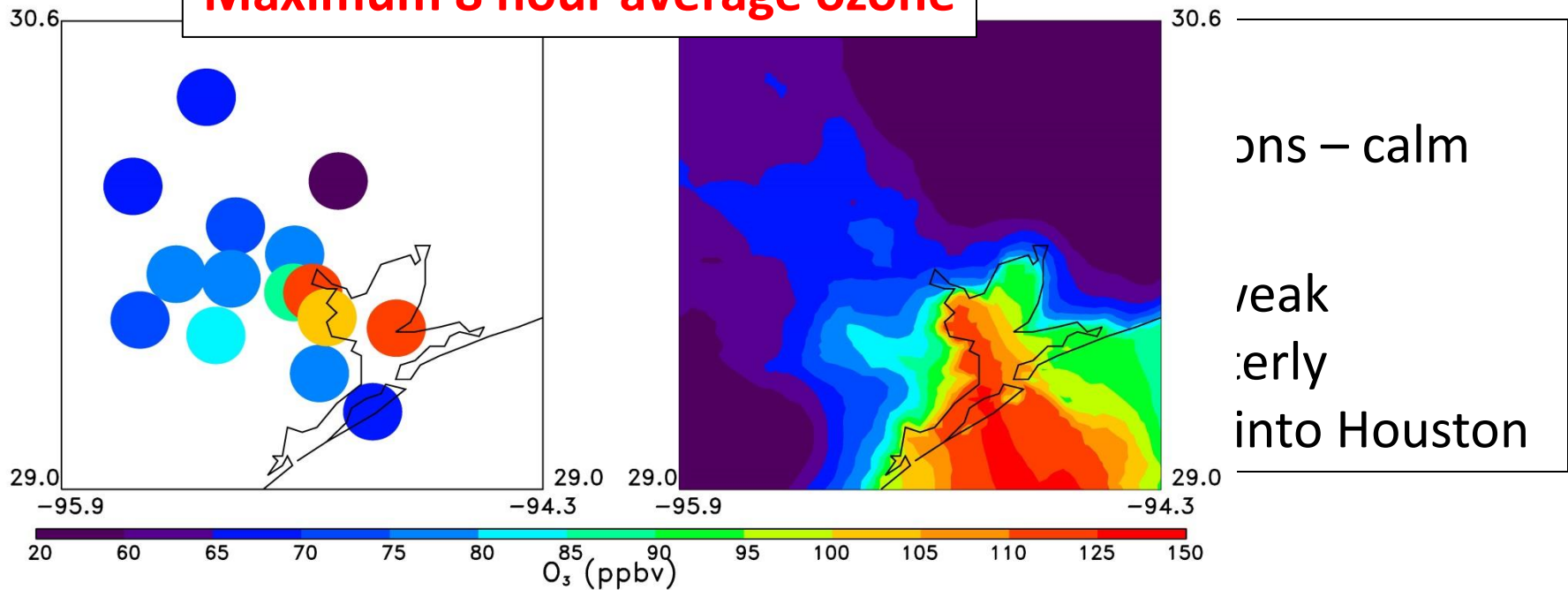


3 pm CST:

Sea and bay breezes pushing inland along Gulf of Mexico shoreline and western coastline of Galveston Bay.

# September 25

**Maximum 8 hour average ozone**



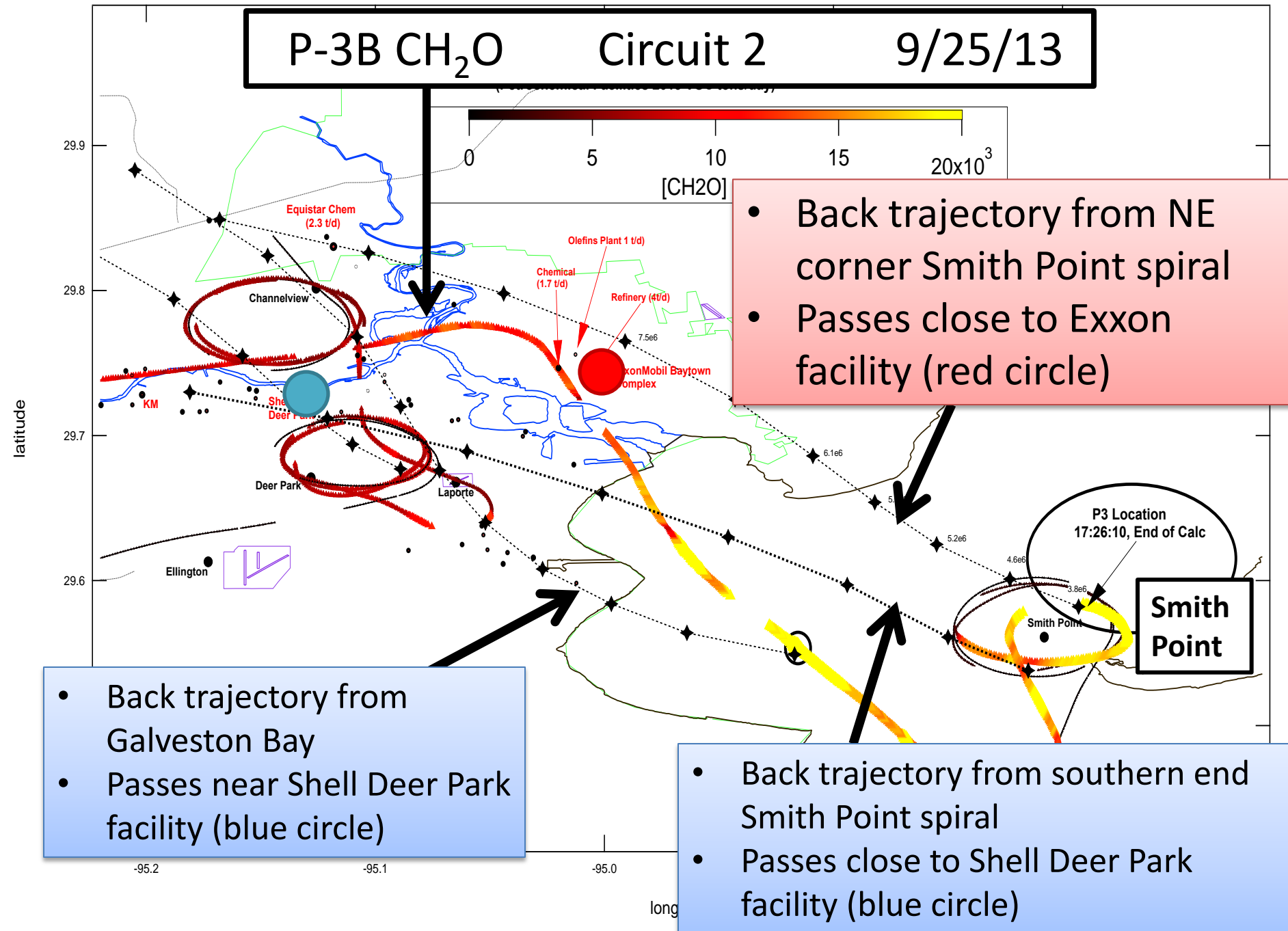
Obs: peak ozone near Galveston Bay.

CMAQ: peak ozone along western coastline of Galveston Bay and Galveston

P-3B CH<sub>2</sub>O

Circuit 2

9/25/13

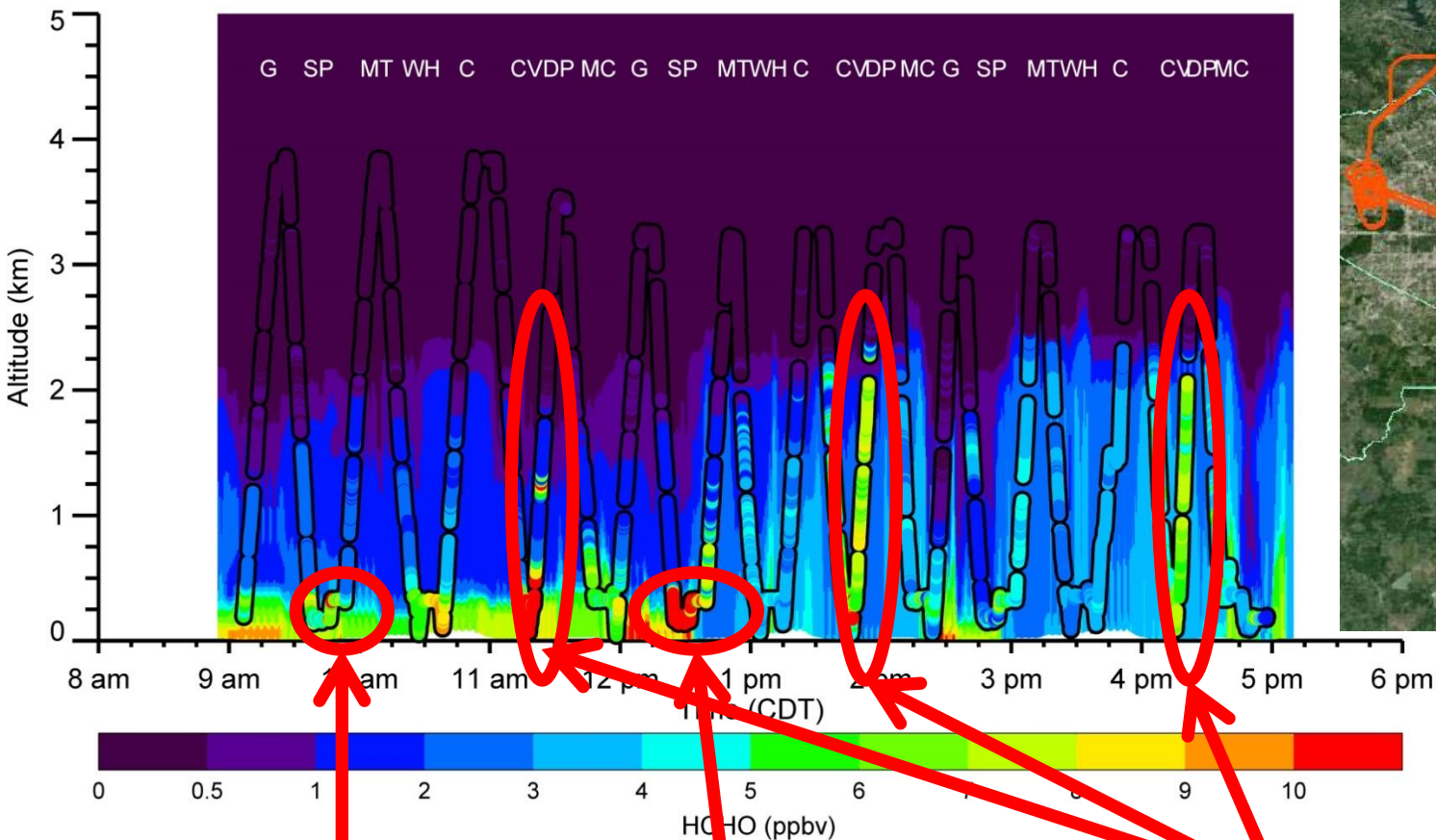


- Back trajectory from NE corner Smith Point spiral
- Passes close to Exxon facility (red circle)

- Back trajectory from Galveston Bay
- Passes near Shell Deer Park facility (blue circle)

- Back trajectory from southern end Smith Point spiral
- Passes close to Shell Deer Park facility (blue circle)

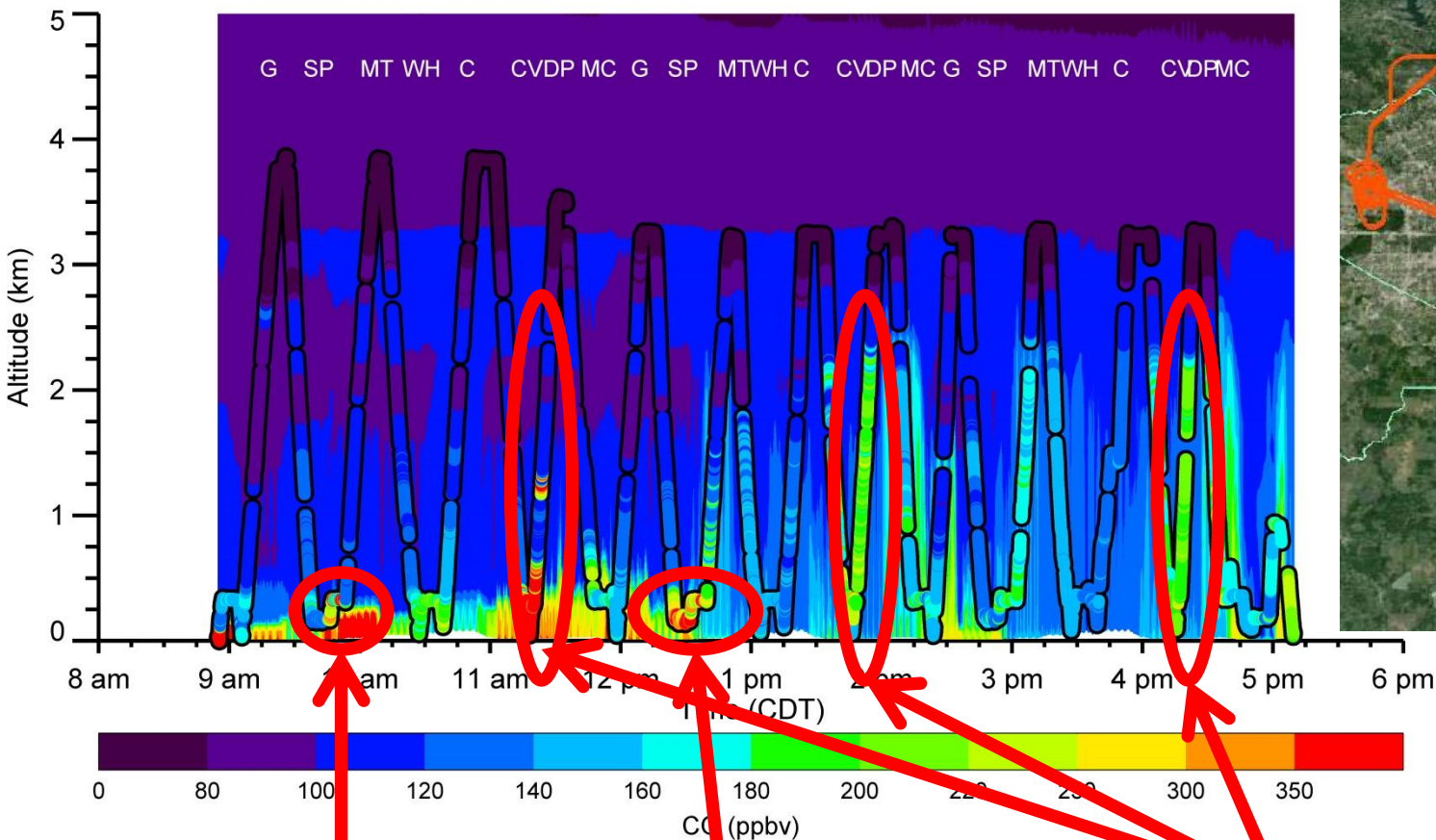




High HCHO  
observed near  
ExxonMobil  
Complex

High HCHO over  
Exxon and  
downwind over  
Smith Point

High HCHO all day  
throughout Deer Park  
spiral

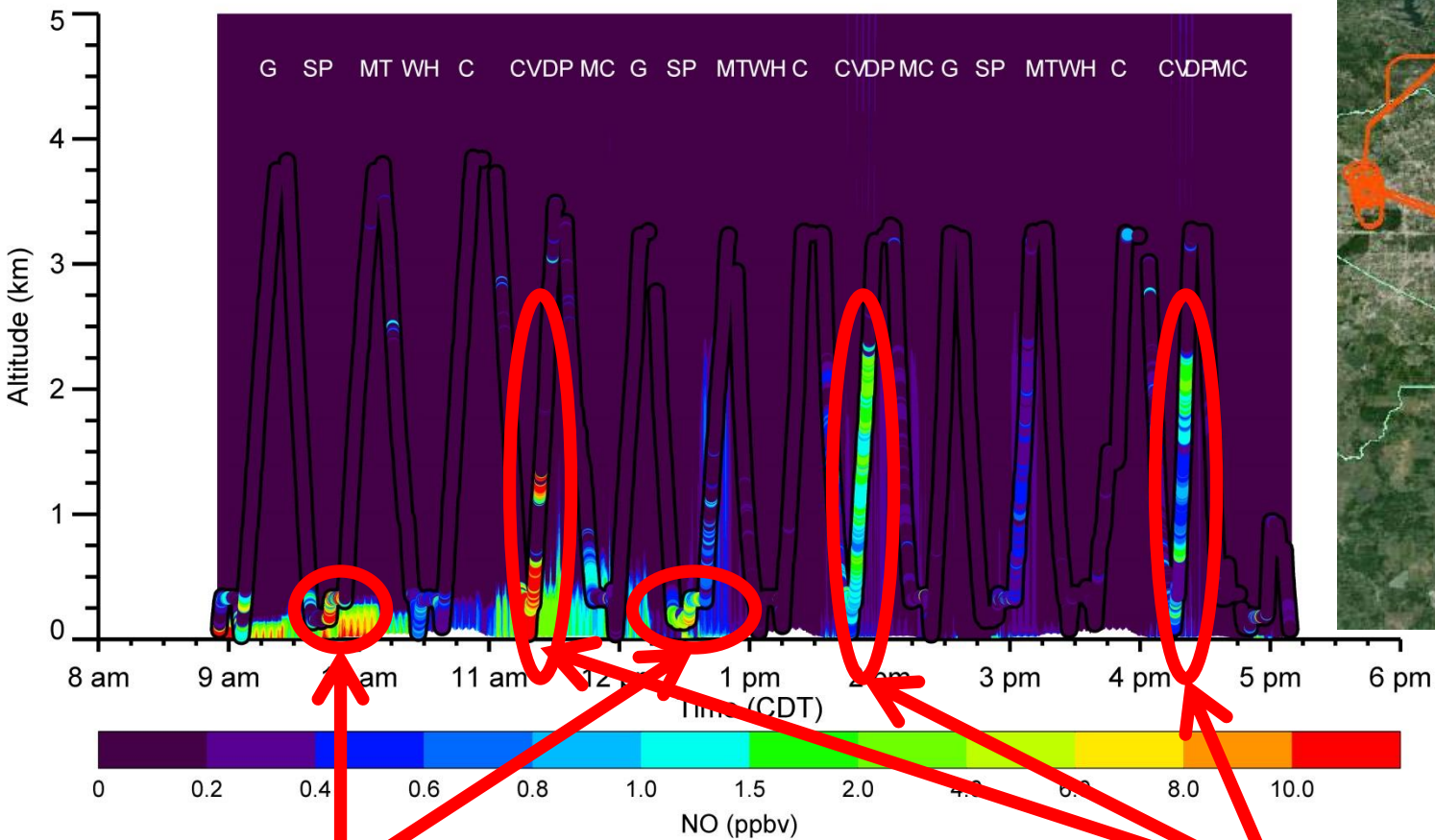


High CO  
observed near  
ExxonMobil  
Complex

High CO over  
Exxon and  
downwind over  
Smith Point

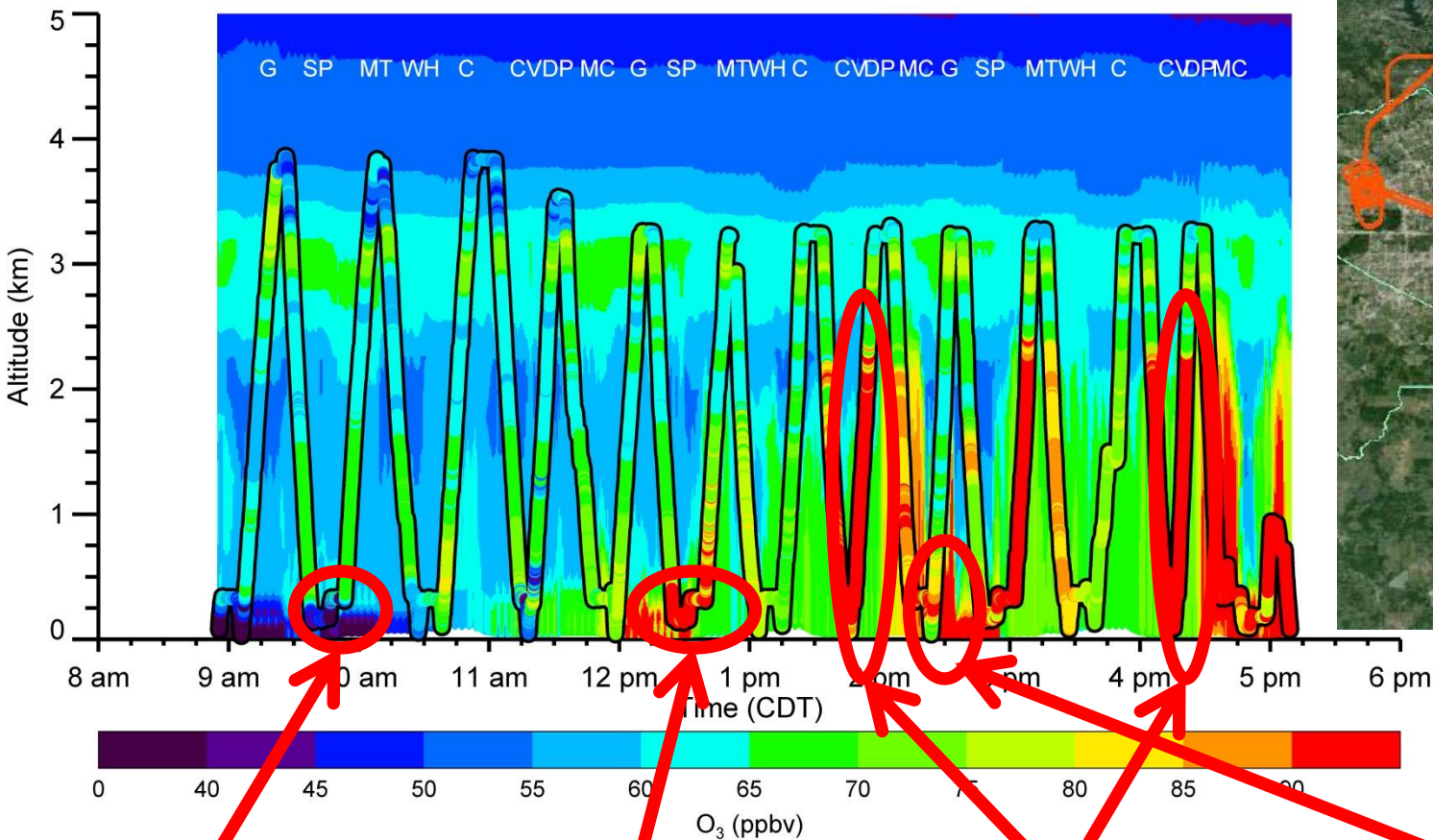
High CO all day  
throughout Deer Park  
spiral





High NO  
observed near  
ExxonMobil  
Complex

High NO all day in the  
Deer Park spiral



Low ozone  
observed near  
ExxonMobil  
Complex

High ozone  
over Exxon  
and downwind  
over Smith  
Point

High ozone during  
the afternoon  
over Deer Park

Low ozone at  
surface and  
high ozone  
aloft over  
Galveston



# Model evaluation

- Meteorology statistics highlight:

- Poor performance of original 4 km simulation
- 2<sup>nd</sup> iterative WRF run is necessary for 1 km horizontal resolution

Sep 24-26	10 m Wind Direction (deg)				
	Orig (4km)	Iter 1 (4 km)	Iter 1 (1 km)	Iter 2 (4 km)	Iter 2 (1 km)
MB	56	37	70	38	38
NMB	39	26	49	26	26
NME	39	26	49	26	26
RMSE	73	55	88	56	55

- Surface ozone statistics highlight:

- Poor performance of original 4 km simulation
- Similar surface ozone results between improved 4 and 1 km CMAQ simulations

Sep 24-26	Surface Ozone (ppbv)		
	Orig (4km)	Iter 2 (4 km)	Iter 2 (1 km)
MB	4.9	2.1	2.9
NMB	15	6.4	8.9
NME	41	29	29
RMSE	17	13	12

# Conclusions

- Improved WRF model run accurately captured the representation of sea and bay breezes. Sea and bay breeze circulations caused pollutants to re-circulate in the area leading to unhealthy air.
- Missing emissions in the inventory, possibly from over-assisted flaring events, resulted in model low bias in surface ozone. However, CMAQ still simulated widespread exceedances of the 8 hour ozone standard indicating over-assisted flaring events made a bad air pollution event worse.
- Improvements in emissions estimates are underway and should lead to improvements in model simulated ozone concentrations.
- Lack of halogen chemistry in CMAQ may be cause of model high ozone bias along Gulf of Mexico coastline. Next release of CMAQ will include halogen chemistry.